DISCONTINUOUS GALERKIN METHODS FOR FLOW AND REACTIVE TRANSPORT

CLINT DAWSON, BÉATRICE RIVIÈRE AND MARY F. WHEELER †

Abstract. The discontinuous Galerkin (DG) metholodogy is a new class of finite elements which are currently being studied by a number of researchers. In this paper we describe two types of discontinuous Galerkin methods for flow and transport problems, with emphasis on applications to porous media.

1. Introduction. Discontinuous Galerkin (DG) methods are a new class of finite element methodology which are being investigated for a wide variety of problems. These methods are based on piecewise polynomial approximating functions, with no assumptions on inter-element continuity. Thus, these methods allow for very general meshes, and also easily allow the user to vary the degree of the approximating polynomial from one element to the next. Hence they are well-suited for so-called $h-p$ adaptivity, where one varies both the mesh and the degree of approximation based on some measure of error. In particular, the DG methods allow for local mesh refinement without the problems associated with "hanging nodes."

The idea of using discontinuous finite element methods with interior penalties on the jumps in the solution can be traced back to the work of Douglas and Dupont [12] and Wheeler [16], among others. These methods were developed for second-order elliptic and parabolic partial differential equations. In the late 1980s and 1990s, DG methods were developed for hyperbolic conservation laws by Cockburn and Shu in a series of papers [5, 8, 9, 10, 7]. More recently, Oden, Babuska and Baumann [13] developed a DG method for steady advection-diffusion equations, very similar to the method derived in [16]. This method has been analyzed and extended by Riviere and Wheeler for elliptic, parabolic and advection-diffusion equations arising in porous media applications [15, 14]. Simultaneously, Cockburn and Shu developed the so-called local discontinuous Galerkin (LDG) method Cockburn and Shu [11] for convection-diffusion equations, based on earlier work by Bassi and Rebay [2] for the compressible Navier-Stokes equations. Dawson and Cockburn then analyzed the LDG method for convection-diffusion equations which arise in the modeling of contaminant transport in porous media [4]. Furthermore, in collaboration with Aizinger and Castillo, we have applied the method to the modeling of nonlinear systems of contaminant transport equations [1].

A review of the history of the DG method and related methods can be found in a recent article by Cockburn, Karniadakis and Shu [6].

In this paper, we will review two DG formulations, discuss some of their theoretical and implementation aspects, and present some numerical results.

2. DG Methods.

2.1. Problem Statement. In this paper, we will consider a flow equation: find a potential p and velocity u, such that

$$\nabla \cdot u = f, \tag{1}$$

$$u = -K\nabla p, \tag{2}$$

where q and K are given data. This equation is coupled to a transport equation for a component concentration c:

$$\phi c_t + \nabla \cdot (uc - D\nabla c) = f, \qquad (x,t) \in \Omega,\ t > 0. \tag{3}$$

The flow problem (1)-(2) is a typical equation arising, for example, in porous media applications, where K is the hydraulic conductivity or ratio of the permeability to the fluid viscosity, and f is

† Center for Subsurface Modeling - C0200; Texas Institute for Computational and Applied Mathematics; The University of Texas at Austin; Austin, TX 78712.

a source/sink term. K may be a function of c. Equation (3) then describes the transport of some chemical species through the porous medium, c is the concentration of the species, ϕ is the porosity of the medium, and D is a velocity-dependent diffusion/dispersion tensor [3]. K and D are positive definite, symmetric matrices, and ϕ is also positive everywhere in the domain. Similar models arise in surface water modeling and atmospheric modeling, the primary difference being that the flow velocity u is determined from the shallow water equations or Navier-Stokes equations.

We solve (1), (2) and (3) on some bounded domain Ω in $\mathbb{R}^d$, and for $t > 0$. Let Γ denote the boundary of Ω, with unit outward normal vector n. For the flow equations we prescribe either the pressure p or the flux $u \cdot n$ on the boundary. Thus

$$p = p_D, \quad \text{on } \Gamma_D, \tag{4}$$
$$u \cdot n = g, \quad \text{on } \Gamma_N. \tag{5}$$

For the transport equation, we partition Γ according to "inflow" and "outflow/noflow" regions, Γ_I and Γ_O, and prescribe

$$(uc - D\nabla c) \cdot n = uc_I \cdot n, \quad \text{on } \Gamma_I, \tag{6}$$
$$(D\nabla c) \cdot n = 0, \quad \text{on } \Gamma_O, \tag{7}$$

where c_I is a specified inflow concentration. Furthermore, we prescribe an initial condition

$$c(x, 0) = c^0(x), \quad \text{on } \Omega. \tag{8}$$

The inflow and outflow/noflow portions of Γ are defined by

$$\Gamma_I = \{x \in \partial\Omega : u \cdot n < 0\}, \tag{9}$$
$$\Gamma_O = \{x \in \partial\Omega : u \cdot n \geq 0\}. \tag{10}$$

2.2. Notation and weak formulation. Let $\{\mathcal{T}_h\}_{h>0}$ denote a family of finite element partitions of $\Omega \subset \mathbb{R}^d$ such that no element Ω_e crosses the boundary of Ω. Let h_e denote the element diameter and h the maximal element diameter. We assume each element Ω_e has a Lipschitz boundary $\partial\Omega_e$. Let $\|\cdot\|_R$ denote the $L^2(R)$ norm. We denote the $L^2(R)$ inner product by $(\cdot,\cdot)_R$, for $R \in \mathbb{R}^d$. To distinguish integration over domains $R \in \mathbb{R}^{d-1}$, e.g., surfaces or lines, we will use the notation $\langle\cdot,\cdot\rangle_R$.

For any smooth function w defined on Ω_e, we denote its trace on $\partial\Omega_e$ from inside Ω_e by w^i, and we denote the trace on $\partial\Omega_e$ from outside Ω_e by w^o. Let γ_l denote an edge in the mesh, and n_l a unit vector normal to the edge, with $n_l = n$ on $\Gamma = \partial\Omega$. Set

$$w^-(x) = \lim_{s\to 0^-} w(x + sn_l), \qquad w^+(x) = \lim_{s\to 0^+} w(x + sn_l),$$

and define

$$\overline{w} = \frac{1}{2}(w^+ + w^-), \qquad [w] = w^+ - w^-.$$

We will describe the DG method of Rivière and Wheeler for the flow problem (1) and (2), and then describe the LDG method for the transport problem (3). However, either method could be used to solve for flow and/or transport.

To motivate the DG method for flow, we combine (1)-(2) into a single equation

$$-\nabla \cdot (K\nabla p) = f. \tag{11}$$

Multiplying (11) by a test function w and integrating by parts over an element Ω_e we find

$$(K\nabla p, \nabla w)_{\Omega_e} - \langle (K\nabla p) \cdot n_e, w^i\rangle_{\partial\Omega_e} = (f, w)_{\Omega_e}, \tag{12}$$

where n_e is the unit outward normal to $\partial\Omega_e$ (note that $n_e = n_l$ or $-n_l$ on each edge). Summing over all elements Ω_e,

$$\sum_e \langle (K\nabla p) \cdot n_e, w^i\rangle_{\partial\Omega_e} = -\sum_l \langle (K\nabla p) \cdot n_l, [w]\rangle_{\gamma_l} + \langle g, w\rangle_{\Gamma_N} + \langle (K\nabla p) \cdot n, w\rangle_{\Gamma_D}, \tag{13}$$

where the summation on l is over interior (non-boundary) edges only. Thus,

$$\sum_e (K\nabla p, \nabla w)_{\Omega_e} + \sum_l \langle (K\nabla p)\cdot n_l, [w]\rangle_{\gamma_l} - \langle (K\nabla p)\cdot n, w\rangle_{\Gamma_D} = \sum_e (f,w)_{\Omega_e} + \langle g, w\rangle_{\Gamma_N}. \tag{14}$$

We motivate the weak formulation used to define the LDG method by rewriting (3) in the following mixed form:

$$\phi c_t + \nabla\cdot(uc+z) = \phi f, \tag{15}$$

$$\tilde{z} = -\nabla c, \tag{16}$$

$$z = D\tilde{z}. \tag{17}$$

and by rewriting the boundary conditions accordingly, that is,

$$(uc+z)\cdot n = (uc_I)\cdot n, \text{ on } \Gamma_I \tag{18}$$

$$z\cdot n = 0, \text{ on } \Gamma_O. \tag{19}$$

We multiply above by arbitrary, smooth test functions w, v and $\tilde{v}$, respectively, and integrate by parts over the element Ω_e to obtain

$$\begin{aligned}&(\phi c_t, w)_{\Omega_e} - (u\,c + z, \nabla w)_{\Omega_e} + \langle (c\,u+z)\cdot n_e, w^i\rangle_{\partial\Omega_e/\Gamma}\\ &+\langle c\,u\cdot n, w^-\rangle_{\Gamma_O} = -\langle c_I\,u\cdot n, w^-\rangle_{\Gamma_I} + (\phi\, f, w)_{\Omega_e},\end{aligned} \tag{20}$$

$$(\tilde{z}, v)_{\Omega_e} - (c, \nabla\cdot v)_{\Omega_e} + \langle c, v^i\cdot n_e\rangle_{\partial\Omega_e} = 0, \tag{21}$$

and

$$(z,\tilde{v})_{\Omega_e} - (D\tilde{z}, \tilde{v})_{\Omega_e} = 0. \tag{22}$$

Here n_e is the unit outward normal to $\partial\Omega_e$.

3. DG and LDG Formulations. Let the approximating space W_h be defined on Ω_e as $\mathcal{P}^{k_e}(\Omega_e)$, the set of all polymonials of degree at most k_e defined on Ω_e.

For the flow equation, we approximate p by $P \in W_h$ using the DG method for $k_e \geq 2$, where P satisfies

$$\begin{aligned}&\sum_e (K\nabla P, \nabla w)_{\Omega_e} + \sum_l \langle (\overline{K\nabla P})\cdot n_l, [w]\rangle_{\gamma_l} - \langle (K\nabla P^-)\cdot n, w\rangle_{\Gamma_D} - \sum_l \langle (\overline{K\nabla w})\cdot n_l, [P]\rangle_{\gamma_l}\\ &\quad + \langle (K\nabla w^-)\cdot n, P^-\rangle_{\Gamma_D} = \sum_e (f,w)_{\Omega_e} + \langle g, w\rangle_{\Gamma_N}. + \langle (K\nabla w^-)\cdot n, p_D\rangle_{\Gamma_D}, \quad \forall w \in W_h.\end{aligned} \tag{23}$$

The first three terms on the left side and the first two terms on the right side of (23) follow directly from (14). The fourth term on the left side is a "penalty" term, note that the true solution p is continuous, thus $[p] = 0$ on γ_l. The other two terms weakly enforce the Dirichlet boundary condition $p = p_D$ on Γ_D.

The LDG method applied to the transport system (20)-(22) is described as follows. We approximate c by $C \in W_h$, z by $Z \in (W_h)^d$, and $\tilde{z}$ by $\tilde{Z} \in (W_h)^d$, where now the degree of the polynomial k_e on any element is ≥ 0. In (20) the value of C and Z across inner element boundaries $\partial\Omega_e$ are approximated by C^u and $\overline{Z}$ respectively, where C^u is the "upwind value" defined as

$$C^u = \begin{cases} C^i, & u\cdot n_e \geq 0, \\ C^o, & u\cdot n_e < 0. \end{cases} \tag{24}$$

Additionally, on Γ_O we approximate C by C^-. In (21), the approximation of C on $\partial\Omega_e$ is $\overline{C}$ on $\partial\Omega_e/\Gamma$ and C^- on Γ.

Incorporating these edge approximations, the LDG method is defined as follows:

$$\sum_e \left[(\phi\, C_t, w)_{\Omega_e} - (u\, C + Z, \nabla w)_{\Omega_e}\right]$$

$$+\sum_l \langle (C^u\, u + \overline{Z}) \cdot n_l, [w]\rangle_{\gamma_l} + \langle C^-\, u \cdot n, w^-\rangle_{\Gamma_O} = \sum_e (f, w)_{\Omega_e} - \langle c_I u \cdot n, w^-\rangle_{\Gamma_I}, \quad \forall w \in W_h, \tag{25}$$

$$\sum_e \left[(\tilde{Z}, v)_{\Omega_e} - (C, \nabla \cdot v)_{\Omega_e}\right] + \sum_l \langle \overline{C}, [v] \cdot n_l\rangle_{\gamma_l} + \langle C^-, v^- \cdot n\rangle_\Gamma = 0, \quad \forall v \in V_h, \tag{26}$$

$$\sum_e \left[(Z, \tilde{v})_{\Omega_e} - (D\tilde{Z}, \tilde{v})_{\Omega_e}\right] = 0, \quad \forall \tilde{v} \in V_h. \tag{27}$$

3.1. Some Remarks on Implementation and Theory. While the LDG method involves three unknowns, in fact the vector quantities Z and $\tilde{Z}$ can be eliminated, giving a system in C unknowns only. In fact, from (26), $\tilde{Z}$ can be eliminated element-by-element in terms of C, and by (27), Z can be eliminated element-by-element in terms of $\tilde{Z}$, and hence in terms of C. Substituting for Z into (25), we end up with a system in C alone.

We have described the LDG method in continuous time. Various time-stepping strategies can be employed, including fully implicit, combinations of explicit/implicit and fully explicit. Some explicit higher-order Runge-Kutta methods for integrating (25) are described in [1].

Because we can employ higher order polynomials, it is possible that near sharp fronts, these polynomials can oscillate. To prevent nonphysical oscillations, we "limit" the higher order terms in the solution through a postprocessing technique. This is done at the end of each step in the calculation. Some limiting techniques are described in [1] and the references therein.

We also remark that one could apply the DG method described above to the diffusion terms in (3), instead of using the LDG formulation. Similarly, one could use the LDG formulation to solve the flow equation.

The schemes above have been analyzed for convergence. Assuming the solution p is sufficient smooth, it has been shown in [14, 15], that the error in the DG method (23) satisfies:

$$||K\nabla P - K\nabla p||_\Omega \le A\frac{h^k}{k^{k-4}}, \tag{28}$$

where A is a constant independent of h and k, where k is the minimum of k_e. In [4], it has been shown that for c sufficiently smooth,

$$\max_{t>0} ||c(\cdot,t) - C(\cdot,t)||_\Omega \le Bh^k, \tag{29}$$

where B is a constant independent of h.

4. Numerical results. The DG method described above has been applied to some typical flow and transport problems in porous media [14]. Below we present results for the DG method applied to flow in the geological L-site, that is located in the south-eastern United States. The L-site consists of a large fly ash disposal pond located adjacent to a river. A cross section of the site is given in Fig.1. There are five different types of rocks. The hydraulic conductivity ranges from 0.31m/day to 17.2m/day. The boundary conditions are the following: no flow on the top and bottom boundaries, and Dirichlet boundary conditions on the vertical boundaries. A constant pressure is imposed at the inlet that is higher than the one at the outlet. Therefore, the flow is driven by a pressure gradient and is expected to be more important in the regions of higher hydraulic conductivity.

First, in Fig. 2 and Fig. 3, we show the quadratic approximation of the pressure first solved on a coarse mesh that consists of distorted quadrilateral elements and second, solved on the mesh that

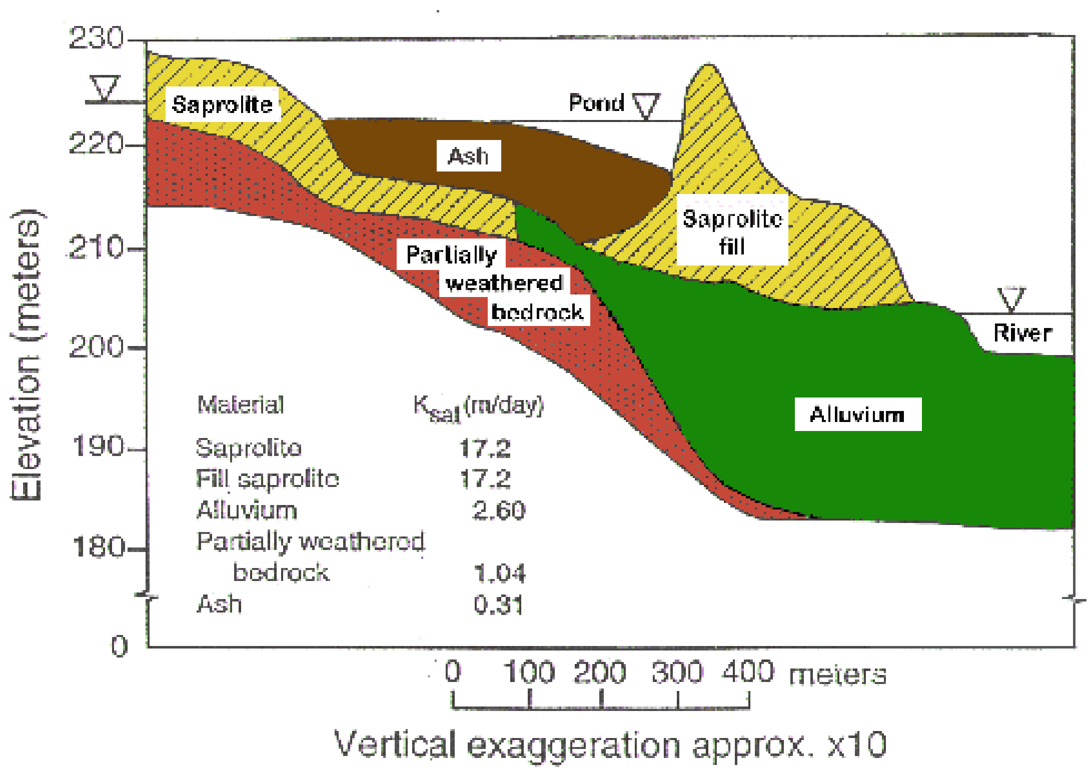

FIG. 1. *Geology of the L-site.*

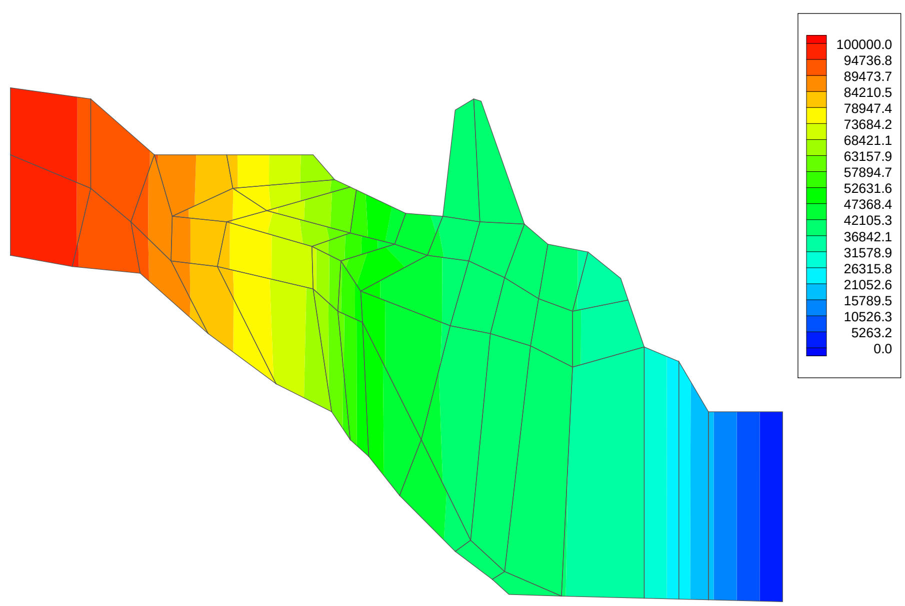

FIG. 2. *Quadratic pressure field on coarse mesh (288 degrees of freedom).*

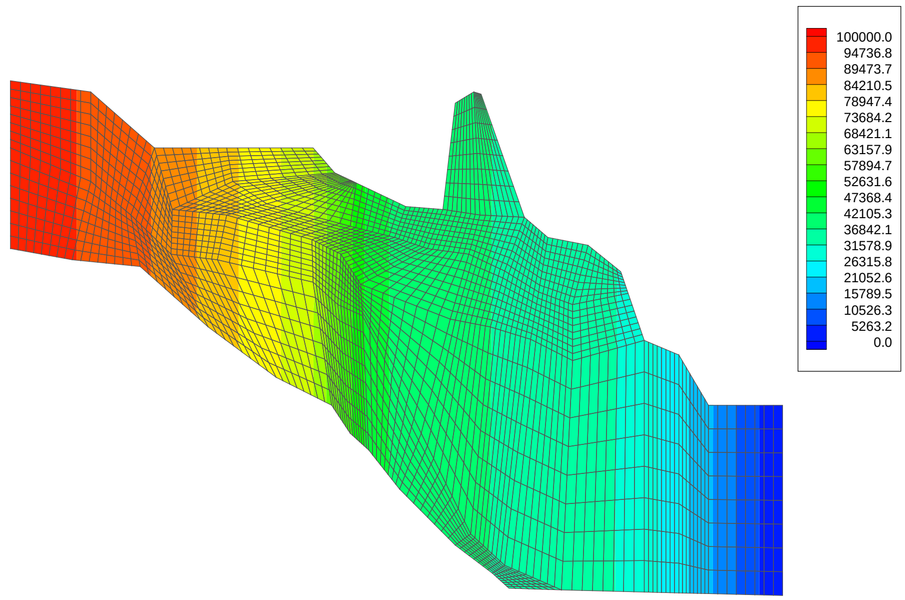

FIG. 3. *Quadratic pressure field on mesh refined three times (18432 degrees of freedom).*

has been uniformly refined. Here, we show that the DG method can handle unstructured meshes and discontinuous coefficients. The velocity fields, obtained by postprocessing the pressure, are shown in Fig. 4 and Fig. 5; as expected, one observes that the Euclidean norm of the velocity is larger in the areas of higher permeability.

The LDG method has been applied to nonlinear systems of equations describing multicomponent contaminant transport [1]. As an example, we consider the system

$$\mathbf{c}_t + \psi(\mathbf{c})_t + u\,\mathbf{c}_x - D\,\mathbf{c}_{xx} = 0, \quad 0 < x < 1, \;\; t > 0, \tag{30}$$

where $u = 1$,

$$\psi(\mathbf{c}) = \begin{pmatrix} \dfrac{c_1}{1 + c_1 + 5\,c_2} \\[2ex] \dfrac{5\,c_2}{1 + c_1 + 5\,c_2} \end{pmatrix}, \tag{31}$$

and the initial and boundary conditions are

$$\mathbf{c}(x,0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad 0 < x < 1, \tag{32}$$

$$\mathbf{c}(0,t) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad t > 0, \tag{33}$$

$$\mathbf{c}(1,t) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad t > 0. \tag{34}$$

This system describes competitive adsorption between two species which are both flowing through the porous medium. The function ψ is a typical Langmuir adsorption isotherm.

In the numerical experiments below we compare results of computations on the same test problem by the LDG method using approximating spaces of different order. First, we test the hyperbolic system obtained from (30) by setting $D = 0$ with the initial and boundary conditions (32)-(34) and isotherm

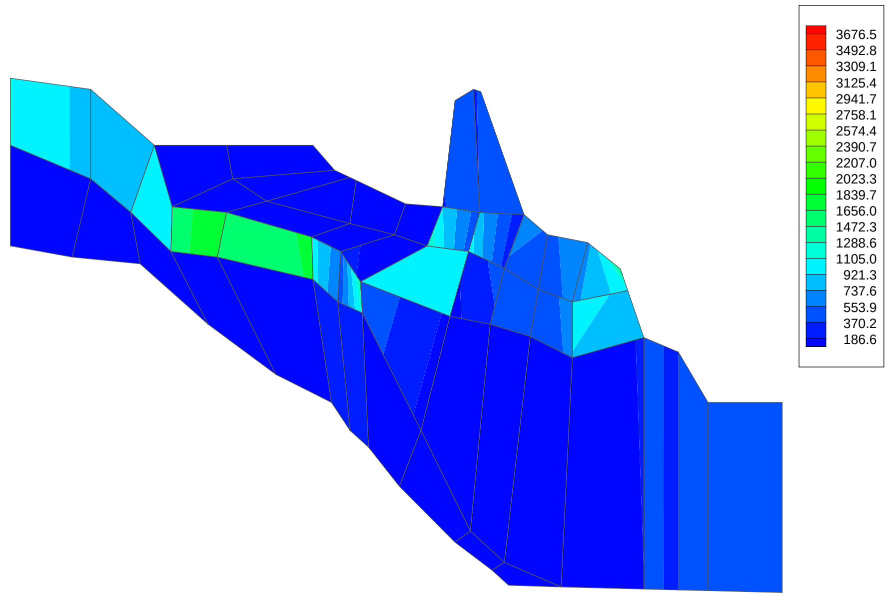

FIG. 4. *Velocity field on coarse mesh (288 degrees of freedom and $r = 2$).*

(31) at the time $T = 0.5$, see Figure 6. Piecewise constant, linear and quadratic approximations were used. Use of piecewise linear approximating polynomials required the local projection procedure to be carried out after each sub time-step, however, as expected the piecewise linear approximation gives us clearly much sharper resolution of the shock wave than the piecewise constant approximation. The piecewise quadratic solution gives very similar results to the piecewise linear solution for this level of resolution. We next conduct a similar test for the parabolic system (30) with $D = 0.01$, the same initial and boundary conditions and the same isotherm as in the previous example. Constants, linear and quadratic approximations are used. In Figure 7, we see that all three approximate solutions lie very close together. In this example, we used different meshes and different time stepping schemes for the different approximations. For constants, we used forward Euler time-stepping, thus the degrees of freedom computed per time step for this solution is 640. For linears we used a second-order Runge-Kutta procedure, thus the degrees of freedom computed per time step is also 160*2*2=640. Similarly, for quadratics a third-order Runge-Kutta procedure was used, requiring the computation of 80*3*3=720 degrees of freedom per time step. In this case, the use of the coarser meshes for linears and quadratics allows for the use of larger time steps. Compared to the constant case, we were able to use a time step four times larger to compute the linear solution, and eight times larger to compute the quadratic solution. This example points out one of the benefits of using higher order polynomials, at least for problems with a sufficient amount of diffusion.

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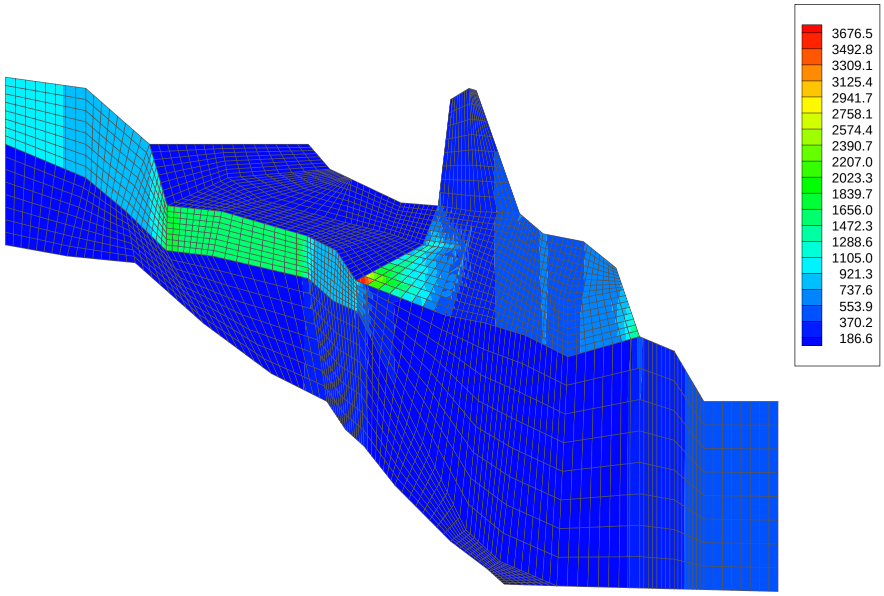

FIG. 5. *Velocity field on mesh refined three times (*18432 *degrees of freedom and* $r = 2$*).*

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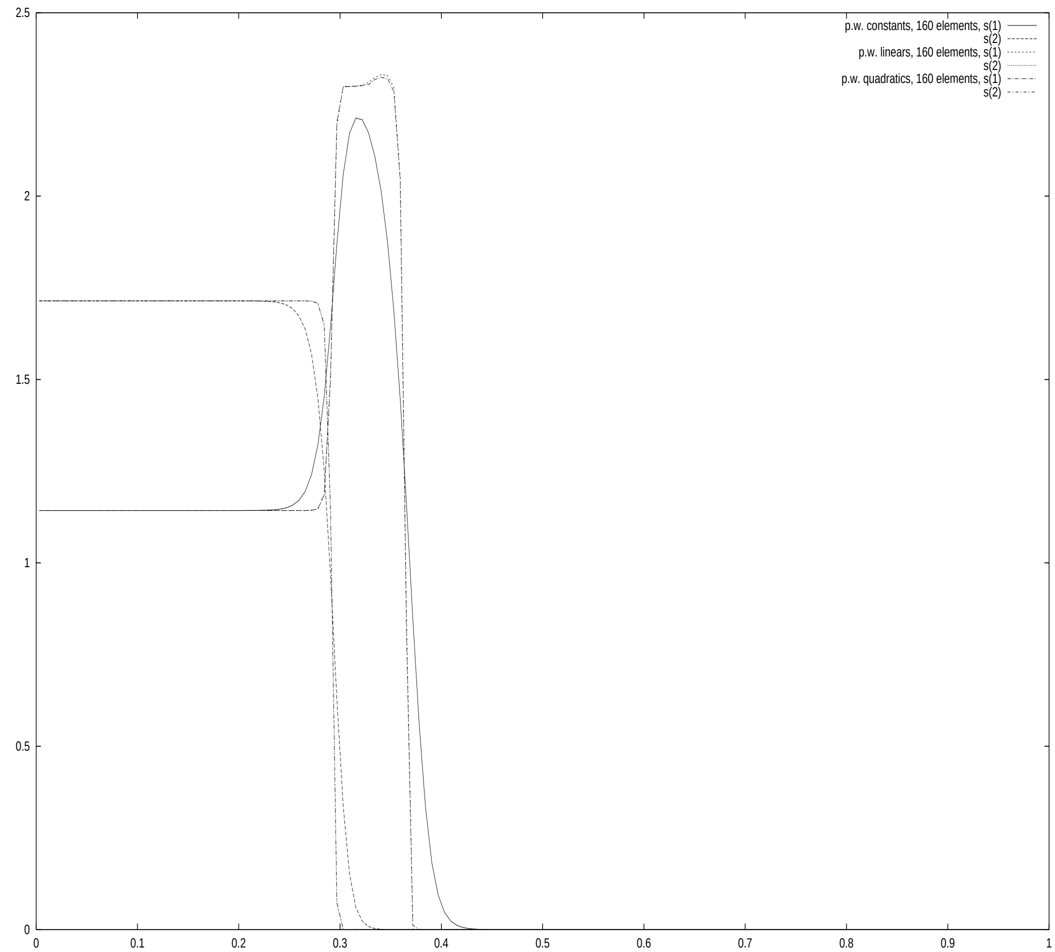

FIG. 6. *Comparison of solutions obtained using different approximating spaces (hyperbolic system)*

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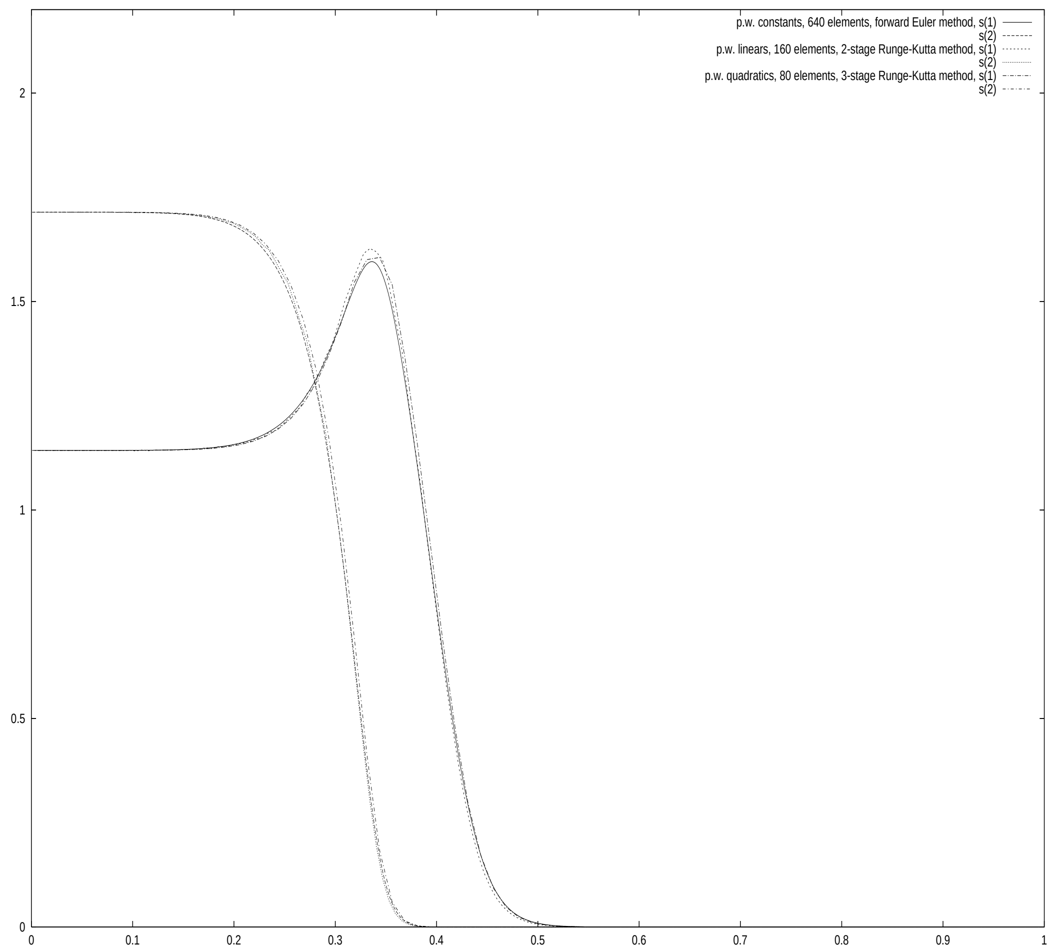

FIG. 7. *Comparison of solutions, obtained using different approximating spaces (parabolic system)*